Modular invariance in the gapped XYZ spin chain

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Abstract. We show that the elliptic parametrization of the coupling constants of the quantum XYZ spin chain can be analytically extended outside of their natural domain, to cover the whole phase-diagram of the model, which is composed of twelve adjacent regions, related to one another by a spin rotation. This extension is based on the modular properties of the elliptic functions and we show how rotations in parameter space correspond to the double covering $PGL(2, \mathbb{Z})$ of the modular group, implying that the partition function of the XYZ chain is invariant under this group in parameter space, in the same way as a Conformal Field Theory partition function is invariant under the modular group acting in real space.

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1. Introduction

The identification of modular properties in integrable theories has always represented a progress in our understanding of the underlying physical and mathematical structures of the model. Modular transformations can appear in a physical model in many different ways. For example, in two-dimensional Conformal Field Theory (CFT) the modular invariance of partition functions on a toroidal geometry [1] has lead to the classification of entire classes of theories [2] and, in many cases, has opened the way to their higher genus investigation, which is a very important tool in applications ranging from strings to condensed matter physics. In a different context, modular transformations are at the root of electromagnetic duality in (supersymmetric) gauge theories [3]. In this case the modular transformations act on the space of parameters of the theory, rather than as space-time symmetries.

In integrable two-dimensional lattice models modular properties were crucial in a Corner Transfer Matrix (CTM) approach [4] to get the so called highest weight probabilities [5, 6]. More recently, the problem of computing bipartite entanglement Renyi entropies (or their Von Neumann limit) in integrable spin chains has been related to the diagonalization of the CTM of the corresponding 2D lattice integrable model. The expressions for these quantities often present a form that can be written in terms of modular functions, like the Jacobi theta functions, suggesting links with a modular theory in the space of parameters. In the XY chain, for example, modular expressions have been found for the entanglement entropy in [7]. Similar modular expressions have been obtained in the calculation [8, 9] of entanglement entropies in the XYZ spin chain, notoriously linked in its integrability to the 8-vertex lattice model [4]. The XYZ model is one of the most widely studied examples of a fully-interacting but still integrable theory, playing the role of a sort of "father" of many other very interesting and useful spin chain models, like the Heisenberg model and its XXZ generalization. Here we would like to start the investigation of its modular symmetries, which – let us stress it again – are not spacetime symmetries, like in CFT, but symmetries in the space of parameters. We believe that the exploiting of modular properties hidden behind the Baxter reparametrization of the XYZ chain can lead, similarly to the aforementioned examples of conformal and gauge theories, to new tools in the investigation of crucial properties of the XYZ chain and its family of related models.

In this paper we show that the XYZ Hamiltonian is invariant under a set of transformations that implement a modular group covering the full plane of parameters of the model in a very specific way. This, in our opinion, prepares the way to the application of the modular group to the study of more complicated quantities, that we plan to investigate in the near future. For instance, this modular invariance may play an important role in a deeper understanding of the Renyi and Von Neumann bipartite entanglement entropies, which are well known to be excellent indicators to detect quantum phase transitions. The paper is organized as follows. In section 2 we recall basic facts about the Hamiltonian formulation of the XYZ spin chain, the

properties of its phase space diagram and the symmetry transformations leading one region of the diagram into another. In section 3 we recall the Baxter solution allowing to relate different portions of the phase space by transformations of the parametrization of the coupling constants of the model in terms of elliptic parameters. Section 4 is devoted to the analytical extension of Baxter solution by switching to new parameters that make the modular properties more evident. This shows how one of the phase space regions can be mapped into the others by applying a modular transformation. The generators of these modular transformations are identified in the next section 5, where the characterization of the actions of the full modular group is described. Our conclusions and outlooks are drawn in section 6.

2. The XYZ chain and its symmetries

The quantum spin-$\frac{1}{2}$ ferromagnetic XYZ chain can be described by the following Hamiltonian

$$\hat{H}_{XYZ} = -\sum_n \left(J_x \sigma_n^x \sigma_{n+1}^x + J_y \sigma_n^y \sigma_{n+1}^y + J_z \sigma_n^z \sigma_{n+1}^z \right) \ , \tag{1}$$

where the σ_n^α $(\alpha = x, y, z)$ are the Pauli matrices acting on the site n, the sum ranges over all sites n of the chain and the constants J_x, J_y and J_z take into account the degree of anisotropy of the model. We assume periodic boundary conditions.

In figure 1 we draw a cartoon of the phase diagram of the XYZ model in the $\left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right)$ plane. We divide it into 12 regions, whose role will become clear as we proceed, named $\mathrm{I}_{a,b,c,}$, $\mathrm{II}_{a,b,c,}$, $\mathrm{III}_{a,b,c,}$. Bold (red-online) continuous lines indicate the gapless phases. To understand better the model, let us first look at the $J_y = J_x$ line. Here we have the familiar XXZ model and we recognize the critical (paramagnetic) phase for $\left|\frac{J_z}{J_x}\right| < 1$ and the (anti-)ferromagnetic Ising phases for $\left|\frac{J_z}{J_x}\right| > 1$. The same physics can be observed for $J_y = -J_x$. There, one can rotate every other spin by 180 degrees around the x-axis to recover a traditional XXZ model. Note, however, that J_z changes sign under this transformation and therefore the ferromagnetic and anti-ferromagnetic Ising phases are reversed. The lines $J_z = \pm J_x$ correspond to a XYX model, i.e. a rotated XXZ model. Thus the phases are the same as before. Finally, along the diagonals $J_y = \pm J_z$ we have a XYY model of the form

$$\hat{H}_{XYY} = -\sum_n \left[J_x \sigma_n^x \sigma_{n+1}^x + J_y \left(\sigma_n^y \sigma_{n+1}^y \pm \sigma_n^z \sigma_{n+1}^z \right) \right] \ . \tag{2}$$

Thus the paramagnetic phase is for $\left|\frac{J_y}{J_x}\right| > 1$ and the Ising phases for $\left|\frac{J_y}{J_x}\right| < 1$, with the plus sign $(J_y = J_z)$ for Ising ferromagnet and the minus $(J_y = -J_z)$ for the anti-ferromagnet.

In this phase diagram we find four *tri-critical points* at $\left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right) = (\pm 1, \pm 1)$. As each paramagnetic phase can be described as a sine-Gordon theory with $\beta^2 = 8\pi$ at the anti-ferromagnetic isotropic point, flowing to a $\beta^2 = 0$ theory at the ferromagnetic

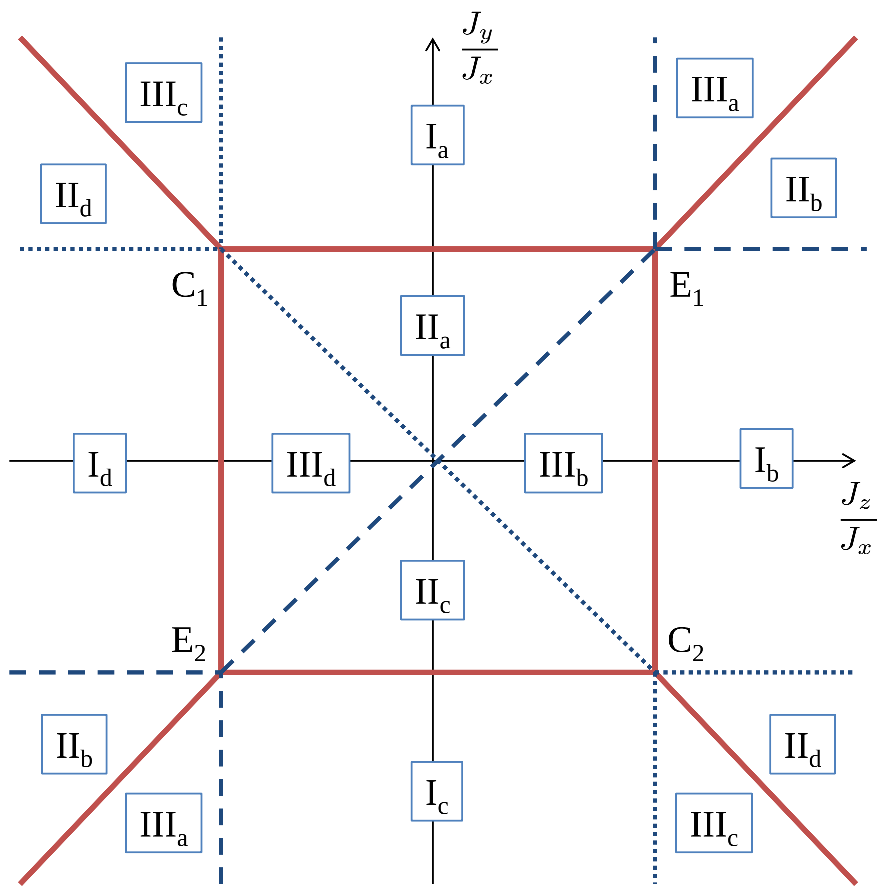

Figure 1. Phase Diagram of the XYZ model in the $\left(\frac{J_y}{J_x}, \frac{J_z}{J_x}\right)$ plane.

Heisenberg point, the critical nature of these tri-critical points is quite different. Assuming $J_x > 0$, at $C_1 = \left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right) = (-1, 1)$ and $C_2 = \left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right) = (1, -1)$ we have two conformal points dividing three equivalent (rotated) sine-Gordon theories with $\beta^2 = 8\pi$. At $E_1 = \left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right) = (1, 1)$ and $E_2 = \left(\frac{J_z}{J_x}, \frac{J_y}{J_x}\right) = (-1, -1)$, we have two $\beta^2 = 0$ points which are no longer conformal, since the low energy excitations have a quadratic spectrum there. The former points correspond to an antiferromagnetic Heisenberg chain at the BKT transition, whilst the latter correspond to an Heisenberg ferromagnet at its first order phase transition. The different nature of the tri-critical points has been highlighted from an entanglement entropy point of view in [9] .

We have seen that the model is invariant under a $\frac{\pi}{2}$ rotation $\mathbf{R}_\alpha = \prod_n \mathrm{e}^{\mathrm{i}\frac{\pi}{4}\sigma_n^\alpha}$ of every spin around one of the axes $\alpha = x, y, z$, followed by the interchange of the couplings $\tilde{\mathbf{R}}_{\beta,\gamma}$ on the perpendicular plane (for instance, for $\alpha = x$, we need $\tilde{\mathbf{R}}_{y,z}\, J_y = J_z$, $\tilde{\mathbf{R}}_{y,z}\, J_z = J_y$). Note that the composition of two rotations, say $\mathbf{R}_y \cdot \mathbf{R}_z$ is compensated by the exchange of the coupling in **opposite** order: $\tilde{\mathbf{R}}_{x,y} \cdot \tilde{\mathbf{R}}_{x,z}$. Similarly, the inversion of every other spin

in a plane $\mathbf{P}_\alpha = \prod_n \sigma^\alpha_{2n}$ can be compensated by changing the signs of the couplings on that plane $\tilde{\mathbf{P}}_{\beta\gamma}$ (where, $\tilde{\mathbf{P}}_{y,z}\, J_y = -J_y$, $\tilde{\mathbf{P}}_{y,z}\, J_z = -J_z$). Three operations are sufficient to generate all these symmetries, for instance $\mathbf{R}_x$, $\mathbf{R}_y$ and $\mathbf{P}_x$ (and $\tilde{\mathbf{R}}_{y,z}$, $\tilde{\mathbf{R}}_{x,z}$ and $\tilde{\mathbf{P}}_{y,z}$).

These generators relate the different regions of the phase diagram: $\mathbf{R}_x \mathrm{I}_a = \mathrm{I}_b$, $\mathbf{R}_y \mathrm{I}_a = \mathrm{III}_a$, $\mathbf{P}_x \mathrm{I}_a = \mathrm{I}_c$ and so on. Note that the action of the $\tilde{\mathbf{R}}_{\alpha,\beta}$ is to exchange the coupling, and we have six different orderings of the three coupling constants. The action of $\tilde{\mathbf{P}}_{y,z}$ additionally doubles the possible phases given by a set of three couplings, giving the total of twelve regions of figure 1. We will show that these operators are equivalent to an extension of the modular group, acting in parameter space.

3. Baxter's solution

The Hamiltonian (1) commutes with the transfer matrices of the zero-field eight vertex model [4] and this means that they can be diagonalized together and they share the same eigenvectors. Indeed, as shown by Sutherland [10], when the coupling constants of the XYZ model are related to the parameters Γ and Δ of the eight vertex model§ at zero external field by the relations

$$J_x : J_y : J_z = 1 : \Gamma : \Delta \ , \tag{3}$$

the row-to-row transfer matrix $\mathbf{T}$ of the latter model commutes with the Hamiltonian $\hat{H}$ of the former. In the principal regime of the eight vertex model it is customary [4] to parametrize the constants Γ and Δ in terms of elliptic functions

$$\Gamma = \frac{1 + k\, \mathrm{sn}^2(\mathrm{i}\lambda; k)}{1 - k\, \mathrm{sn}^2(\mathrm{i}\lambda; k)} \ , \qquad \Delta = -\frac{\mathrm{cn}(\mathrm{i}\lambda; k)\, \mathrm{dn}(\mathrm{i}\lambda; k)}{1 - k\, \mathrm{sn}^2(\mathrm{i}\lambda; k)} \ , \tag{4}$$

where $\mathrm{sn}(z;k)$, $\mathrm{cn}(z;k)$ and $\mathrm{dn}(z;k)$ are Jacoby elliptic functions of parameter k, while λ and k are the argument and the parameter (respectively) whose natural regimes are

$$0 \le k \le 1 \ , \qquad 0 \le \lambda \le K(k') \ , \tag{5}$$

$K(k')$ being the complete elliptic integral of the first kind (A.7) of argument $k' = \sqrt{1-k^2}$.

In light of (3), without loss of generality, we rescale the energy and set $J_x = 1$. We recall that the parametrization (4) of the parameters is particularly suitable to describe an anti-ferroelectric phase of the eight vertex model, corresponding to $\Delta \le -1$, $|\Gamma| \le 1$. However, using the symmetries of the model and the freedom under the rearrangement of parameters, it can be used in all cases by re-defining the relations that hold between Δ and Γ and the Boltzmann weights (for more details see [4]). We can apply the same procedure to extract the physical parameters of the XYZ model in the whole of the

§ We adopt the conventions of [4] on the relation among Γ, Δ and the Boltzmann weights of the XYZ chain.

phase diagram in a fairly compact way. In fact, when $|J_y| < 1$ and $|J_z| < 1$ we have:

$$\begin{cases} \Gamma &= \dfrac{|J_z - J_y| - |J_z + J_y|}{|J_z - J_y| + |J_z + J_y|} , \\ \Delta &= -\dfrac{2}{|J_z - J_y| + |J_z + J_y|} , \end{cases} \tag{6}$$

while for $|J_y| > 1$ or $|J_z| > 1$, we get:

$$\begin{cases} \Gamma &= \dfrac{\min\left[1, \left|\frac{|J_z - J_y| - |J_z + J_y|}{2}\right|\right]}{\max\left[1, \left|\frac{|J_z - J_y| - |J_z + J_y|}{2}\right|\right]} \cdot \operatorname{sgn}\Big(|J_z - J_y| - |J_z + J_y| \Big) , \\ \\ \Delta &= -\dfrac{1}{2} \dfrac{|J_z - J_y| + |J_z + J_y|}{\max\left[1, \left|\frac{|J_z - J_y| - |J_z + J_y|}{2}\right|\right]} , \end{cases} \tag{7}$$

where Γ and Δ are given by (4). For instance, for $|J_y| \leq 1$ and $J_z \leq -1$ we recover $J_y = \Gamma$ and $J_z = \Delta$, while for $J_y \geq 1$ and $|J_z| \leq 1$ we have $J_y = -\Delta$ and $J_z = -\Gamma$. In figure 1 we show the phase diagram divided in the different regions where a given parametrization applies.

While Baxter's procedure allows to access the full phase-diagram of the model, it introduces artificial discontinuities at the boundaries between the regions, as indicated by the *max* and *min* functions and the associated absolute values. In the next section we will show that, with a suitable analytical continuation of the elliptic parameters, we can extend the parametrization of a given region to the whole phase diagram in a continuous way, which numerically coincides with Baxter's prescription.

4. Analytical extension of Baxter's solution

To streamline the computation, it is convenient to perform a Landen transformation on (4) and to switch to new parameters (u, l)

$$l \equiv \frac{2\sqrt{k}}{1+k} , \qquad u \equiv (1+k)\lambda , \tag{8}$$

so that‖

$$\Gamma = \frac{1 + k \operatorname{sn}^2(\mathrm{i}\lambda; k)}{1 - k \operatorname{sn}^2(\mathrm{i}\lambda; k)} = \frac{1}{\operatorname{dn}(\mathrm{i}u; l)} , \tag{9}$$

$$\Delta = -\frac{\operatorname{cn}(\mathrm{i}\lambda; k) \operatorname{dn}(\mathrm{i}\lambda; k)}{1 - k \operatorname{sn}^2(\mathrm{i}\lambda; k)} = -\frac{\operatorname{cn}(\mathrm{i}u; l)}{\operatorname{dn}(\mathrm{i}u; l)} . \tag{10}$$

The natural domain of (λ, k) corresponds to

$$0 \leq u \leq 2K(l') \qquad 0 \leq l \leq 1 . \tag{11}$$

We also have the following identities

$$l' = \sqrt{1 - l^2} = \frac{1-k}{1+k} , \qquad K(l) = (1+k)K(k) , \qquad K(l') = \frac{1+k}{2} K(k') , \tag{12}$$

‖ See, for instance, table 8.152 of [20]

from which it follows that the Landen transformation doubles the elliptic parameter $\tau(k) = \mathrm{i}\frac{K(k')}{K(k)} = 2\mathrm{i}\frac{K(l')}{K(l)} = 2\tau(l)$.

Using (A.14)) we have

$$l = \sqrt{\frac{1-\Gamma^2}{\Delta^2-\Gamma^2}} \ . \tag{13}$$

Furthermore, elliptic functions can be inverted in elliptic integrals and from (10) we have

$$\mathrm{i}u = \int_{-1}^{-\Gamma} \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-l'^2t^2)}} = \mathrm{i}\Big[K(l') - F(\arcsin\Gamma; l')\Big] \ . \tag{14}$$

Together, (13, 14) invert (9, 10) and, together with (6, 7), give the value of Baxter's parameters for equivalent points of the phase diagram. It is important to notice that these identities ensure that the domain (11) maps into $|\Gamma| \leq 1$ and $\Delta \leq -1$ and vice-versa.

The idea of the analytical continuation is to use (13) to extend the domain of l beyond its natural regime. To this end, let us start from a given region, let say I_a in fig. 1, with $|J_z| \leq 1$ and $J_y \geq 1$. By (7) we have:

$$J_y(u,l) = -\Delta = \frac{\mathrm{cn}(\mathrm{i}u;\, l)}{\mathrm{dn}(\mathrm{i}u;\, l)} \ , \qquad J_z(u,l) = -\Gamma = -\frac{1}{\mathrm{dn}(\mathrm{i}u;\, l)} \ , \tag{15}$$

and thus

$$l = \sqrt{\frac{1-J_z^2}{J_y^2-J_z^2}} \ , \qquad \mathrm{i}u = \int_{-1}^{J_z} \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-l'^2t^2)}} \ . \tag{16}$$

Notice that within region I_a we can recast the second identity as

$$u = K(l') + F(\arcsin J_z; l') \ , \tag{17}$$

which makes z explicitly real and $0 \leq u \leq 2K(l')$.

We now take (16) as the definition of l and use it to extend it over the whole phase diagram. For instance, in region II_a ($0 \leq J_y \leq 1$, $J_z^2 \leq J_y^2$), using (16) we find $l > 1$. To show that this analytical continuation gives the correct results, we write $l = 1/\tilde{l}$, so that $0 \leq \tilde{l} \leq 1$ and use (A.32) in (15), which gives

$$J_y(u,l) = \frac{\mathrm{dn}(\mathrm{i}\tilde{u};\, \tilde{l})}{\mathrm{cn}(\mathrm{i}\tilde{u};\, \tilde{l})} \ , \qquad J_z(u,l) = -\frac{1}{\mathrm{cn}(\mathrm{i}\tilde{u};\, \tilde{l})} \ , \tag{18}$$

which reproduces Baxter's definitions in (6): $\Gamma = -\frac{J_z}{J_y}$, $\Delta = -\frac{1}{J_y}$. Note that we also rescale the argument $\tilde{u} = lu$, so that $0 \leq \tilde{u} \leq 2K(\tilde{l}')$. This shows that we can use (15) to cover both regions I_a and II_a, by letting $0 \leq l < \infty$ (note that $l = 1$ corresponds to the boundary between the two regions).

We can proceed similarly for the rest of the phase diagram. However, the second part of (16) needs some adjustment. Since elliptic integrals are multivalued functions of their parameters, to determine the proper branch of the integrand one starts in the

principal region and follows the analytical continuation. The result of this procedure can be summarized as

$$\begin{aligned} \mathrm{i}u &= \mathrm{i}\Big[K(l') + F(\arcsin J_z; l')\Big] + \Big[1 - \mathrm{sign}(J_y)\Big]K(l) \\ &= F(\arcsin J_y; l) - K(l) + \mathrm{i}\Big[1 + \mathrm{sign}(J_z)\Big]K(l') \ , \end{aligned} \tag{19}$$

where all the elliptic integrals here are taken at their principal value. We did not find a single parametrization without discontinuities in the whole phase diagram. Close to $J_z \simeq 0$, the first line of (19) is continuous, while the second has a jump. The opposite happens for $J_y \simeq 0$, but, due to the periodicity properties of (9, 10), both expressions are proper inversions of (15) valid everywhere.

Thus, we accomplished to invert (15) and to assign a pair of (u, l) to each point of the phase diagram (J_y, J_z), modulo the periodicity in u space. The analysis of these mappings shows an interesting structure. From (16) it follows that that regions I's have $0 \leq l \leq 1$, while II's have $l \geq 1$, which can be written as $l = 1/\tilde{l}$, with $0 \leq \tilde{l} \leq 1$. Finally, regions III's have purely imaginary $l = \mathrm{i}\,\tilde{l}/\tilde{l}'$, with $0 \leq \tilde{l} \leq 1$. In each region, the argument runs along one of the sides of a rectangle in the complex plane of sides $2K(\tilde{l})$ and $\mathrm{i}2K(\tilde{l}')$. Thus, we can write

$$J_y(z, l) = \frac{\mathrm{cn}(\zeta\, u(z);\, l)}{\mathrm{dn}(\zeta\, u(z);\, l)} \ , \qquad J_z(u, l) = \frac{1}{\mathrm{dn}(\zeta\, u(z);\, l)} \ , \qquad 0 \leq z \leq \pi \ , \tag{20}$$

where $\zeta = 1, \tilde{l}, \tilde{l}'$ in regions I's, II's, and III's respectively. Moreover, $u(z) = \mathrm{i}(\pi - z)\frac{2}{\pi}K(\tilde{l}')$ for regions of type a; $u(z) = (\pi - z)\frac{2}{\pi}K(\tilde{l})$ for type b's; $u(z) = 2K(\tilde{l}) + \mathrm{i}z\frac{2}{\pi}K(\tilde{l}')$ for regions of type c; and $u(z) = \mathrm{i}2K(\tilde{l}') + z\frac{2}{\pi}K(\tilde{l})$ for regions of type d. In figure 2 we draw these four paths for the argument and the directions of the primary periods of the elliptic functions for regions of type I, II, and III. Figure 3 shows the contour lines of (u, l) in (J_y, J_z) plane, as given by (20).

It is known that only purely real or purely imaginary arguments (modulo a half periodicity) ensure the reality of an elliptic function (and thus that the coupling constant are real and the Hamiltonian hermitian). We will show that this regular structure is actually connected with the symmetries of the model. The validity of this analytical continuation is checked, like we just did for region II_a, using the relations connecting elliptic functions of different elliptic parameters (see Appendix A or [21]). These relations are rooted in the modular invariance of the torus on which elliptic functions are defined. In the next section, we are going to show explicitly the action of the modular group, in covering the phase diagram of the XYZ model.

Before we proceed, we remark that, while it is possible that the validity of Baxter parametrization outside of its natural domain has been observed before by other author's analysis, we did not find any reference to it in the literature and we believe that we are the first to show in details how to construct the complete extension to the whole phase diagram, which is condensed in Table 1 in the next section.

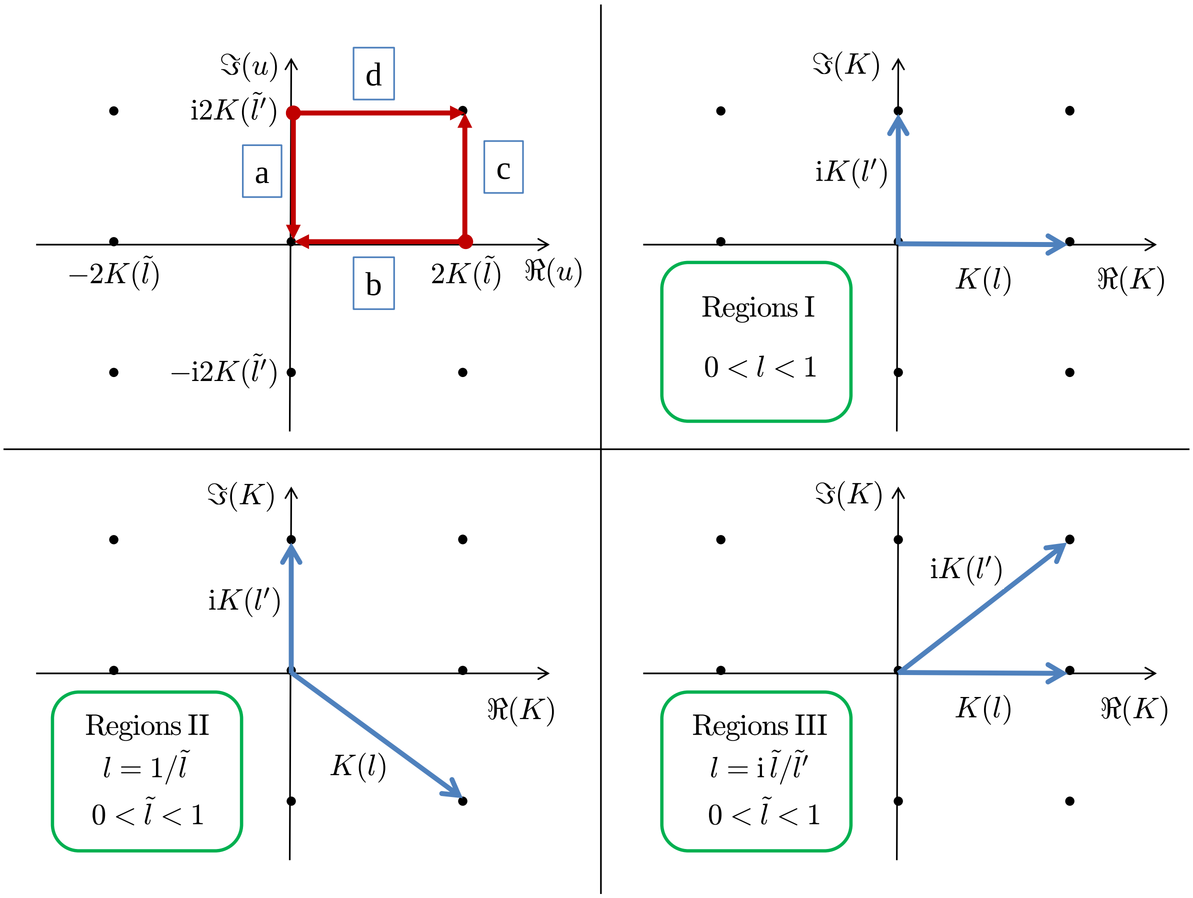

Figure 2. On the top left, in regions of type a, b, c, and d, the argument of the elliptic functions runs along one of the sides of the rectangle. In the remaining quadrants, the directions of the quater-periods $K(l)$ and $\mathrm{i}K(l')$ in I, II, and III regions.

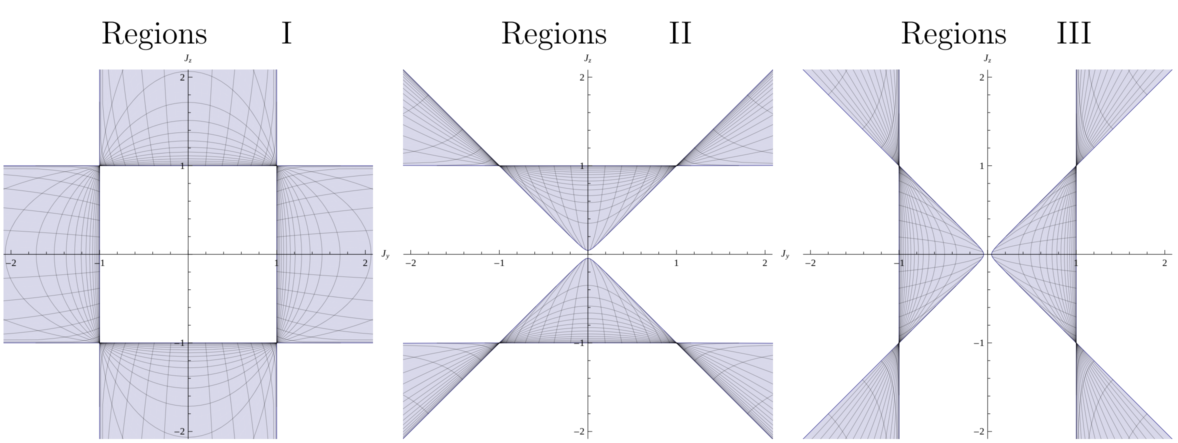

Figure 3. Contour plots of the (u, l) lines in the different regions of the phase diagram, as given by (20).

5. The action of the modular group

In the previous section, we showed that Baxter's parametrization of the parameters of the XYZ chain can be analytically extended outside of the principal regime to cover the whole phase-diagram and thus that any path in the real two-dimensional (J_y, J_z)-space corresponds to a continuous path of (u, l) in $\mathbb{C}^2$. This extension is due to the fact that the analytical continuation of elliptic functions in the complex plane can be related to the action of the modular group. We refer to [21] for a detail explanation of the relation between elliptic functions and the modular group and to Appendix A for a collection of useful identities.

Points related by a modular transformations correspond to the same (Γ, Δ) point in the mapping to the eight-vertex model (6,7). We now want to show that the modular group can be connected to the symmetries of the model that we discussed in the introduction. Let us start again in region $\mathrm{I_a}$, but to make the modular structure more apparent, this time let us write the parametrization in terms of theta functions using (A.6)

$$J_y = \frac{\theta_3(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2\left[(z-\pi)\tau|\tau\right]}{\theta_3\left[(z-\pi)\tau|\tau\right]} , \qquad J_z = \frac{\theta_3(0|\tau)}{\theta_4(0|\tau)} \frac{\theta_4\left[(z-\pi)\tau|\tau\right]}{\theta_3\left[(z-\pi)\tau|\tau\right]} , \tag{21}$$

where $0 \le z \le \pi$, and we used (A.4).

As the Jacobi elliptic functions are doubly-periodic, the torus on which they are defined can be viewed as the quotient $\mathbb{C}/\mathbb{Z}^2$. In region $\mathrm{I_a}$, for $0 \le l \le 1$, the fundamental domain is the rectangle with sides on the real and imaginary axis, of length respectively $\omega_1 = 4K(l)$ and $\omega_3 = \mathrm{i}4K(l')$, and the path followed by z is a half-period along the imaginary axis. A modular transformation turns the rectangle into a parallelogram constructed on the same two-dimensional lattice, but leaves the path of the argument untouched. To this end, we extend the representation of the modular group to keep track of the original periods and introduce the two vectors σ_R and σ_I, which points along the original real and imaginary axis. In $\mathrm{I_a}$, these two vectors are $\sigma_R = \frac{\omega_1}{\omega_1} = 1$ and $\sigma_I = \frac{\omega_3}{\omega_1} = \tau$ (we remind that, when using theta functions, every length is normalized by the periodicity on the real axis, i.e. ω_1). We will also need to extend the modular group and thus we introduce the additional complex number $\phi = -\pi\sigma_I$, which is a sort of an initial phase in the path of the argument.

With these definitions, we write (21) as

$$J_y = \frac{\theta_3(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2\left[z\,\sigma_I + \phi|\tau\right]}{\theta_3\left[z\,\sigma_I + \phi|\tau\right]} , \qquad J_z = \frac{\theta_3(0|\tau)}{\theta_4(0|\tau)} \frac{\theta_4\left[z\,\sigma_I + \phi|\tau\right]}{\theta_3\left[z\,\sigma_I + \phi|\tau\right]} . \tag{22}$$

The two generators of the modular group act on this extended representation as

$$\mathbf{T} \begin{pmatrix} \tau \\ \sigma_R \\ \sigma_I \\ \phi \end{pmatrix} = \begin{pmatrix} \tau+1 \\ \sigma_R \\ \sigma_I \\ \phi \end{pmatrix} , \qquad \mathbf{S} \begin{pmatrix} \tau \\ \sigma_R \\ \sigma_I \\ \phi \end{pmatrix} = \begin{pmatrix} -\frac{1}{\tau} \\ -\frac{\sigma_R}{\tau} \\ -\frac{\sigma_I}{\tau} \\ -\frac{\phi}{\tau} \end{pmatrix} . \tag{23}$$

A general modular transformation which gives $\tau' = \frac{c+d\,\tau}{a+b\,\tau}$ also does

$$\sigma_R \to \frac{1}{a+b\,\tau} = d - b\,\tau' \,, \qquad \sigma_I \to \frac{\tau}{a+b\,\tau} = -c + a\,\tau' \,, \qquad \phi \to \frac{\phi}{a+b\,\tau} \,, \quad (24)$$

i.e. it expresses the original real and imaginary periods in terms of the two new periods.

For instance, applying the $\mathbf{S}$ transformation $\mathbf{S}\tau = \tau_S = -\frac{1}{\tau}$ to region $\mathrm{I_a}$ we have

$$\mathbf{S}J_y = \frac{\theta_3(0|\tau_S)}{\theta_2(0|\tau_S)} \frac{\theta_2\left[z-\pi|\tau_S\right]}{\theta_3\left[z-\pi|\tau_S\right]} = \frac{\theta_3(0|\tau)}{\theta_4(0|\tau)} \frac{\theta_4\left[(z-\pi)\tau|\tau\right]}{\theta_3\left[(z-\pi)\tau|\tau\right]} = J_z \,, \quad (25a)$$

$$\mathbf{S}J_z = \frac{\theta_3(0|\tau_S)}{\theta_4(0|\tau_S)} \frac{\theta_4\left[z-\pi|\tau_S\right]}{\theta_3\left[z-\pi|\tau_S\right]} = \frac{\theta_3(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2\left[(z-\pi)\tau|\tau\right]}{\theta_3\left[(z-\pi)\tau|\tau\right]} = J_y \,, \quad (25b)$$

which is equivalent to the Baxter's elliptic parametrization of region I_b and shows that

$$\mathbf{S} = \tilde{\mathbf{R}}_{y,z} = \mathbf{R}_x \,. \quad (26)$$

The other generator of the modular group $\mathbf{T}\tau = \tau_T = \tau + 1$ gives

$$\mathbf{T}J_y = \frac{\theta_3(0|\tau_T)}{\theta_2(0|\tau_T)} \frac{\theta_2\left[(z-\pi)\tau|\tau_T\right]}{\theta_3\left[(z-\pi)\tau|\tau_T\right]} = \frac{\theta_4(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2\left[(z-\pi)\tau|\tau\right]}{\theta_4\left[(z-\pi)\tau|\tau\right]} = \frac{J_y}{J_z} \,, \quad (27a)$$

$$\mathbf{T}J_z = \frac{\theta_3(0|\tau_T)}{\theta_4(0|\tau_T)} \frac{\theta_4\left[(z-\pi)\tau|\tau_T\right]}{\theta_3\left[(z-\pi)\tau|\tau_T\right]} = \frac{\theta_4(0|\tau)}{\theta_3(0|\tau)} \frac{\theta_3\left[(z-\pi)\tau|\tau\right]}{\theta_4\left[(z-\pi)\tau|\tau\right]} = \frac{1}{J_z} \,, \quad (27b)$$

which maps I_a into region III_a, in agreement with (7) and gives

$$\mathbf{T} = \tilde{\mathbf{R}}_{x,z} = \mathbf{R}_y \,, \quad (28)$$

as can be seen by rescaling the couplings J_x, J_y, and J_z by $1/J_z$.

Finally, we introduce an additional operator $\mathbf{P}$:

$$\mathbf{P} \begin{pmatrix} \tau \\ \sigma_R \\ \sigma_I \\ \phi \end{pmatrix} = \begin{pmatrix} \tau \\ \sigma_R \\ \sigma_I \\ \phi + \pi\left[\sigma_R + \sigma_I\right] \end{pmatrix} \,, \quad (29)$$

which shifts by half a period in both directions the origin of the path of the argument. Applying it to I_a gives

$$\mathbf{P}J_y = \frac{\theta_3(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2\left[z\tau+\pi|\tau\right]}{\theta_3\left[z\tau+\pi|\tau\right]} = -J_y \,, \quad (30a)$$

$$\mathbf{P}J_z = \frac{\theta_3(0|\tau)}{\theta_4(0|\tau)} \frac{\theta_4\left[z\tau+\pi|\tau\right]}{\theta_3\left[z\tau+\pi|\tau\right]} = -J_z \,, \quad (30b)$$

which covers I_c and leads to the identification

$$\mathbf{P} = \tilde{\mathbf{P}}_{y,z} = \mathbf{P}_x \,. \quad (31)$$

The three operation $\mathbf{T}$, $\mathbf{S}$ and $\mathbf{P}$, with:

$$(\mathbf{S}\cdot\mathbf{T})^3 = \mathbb{I} \,, \qquad \mathbf{S}^2 = \mathbb{I} \,, \qquad \mathbf{P}^2 = \mathbb{I} \,, \qquad \mathbf{P}\cdot\mathbf{S} = \mathbf{S}\cdot\mathbf{P} \,, \qquad \mathbf{P}\cdot\mathbf{T} = \mathbf{T}\cdot\mathbf{P} \,. \quad (32)$$

Region	Modular Generator	σ_R	σ_I	ϕ	τ	l	Region	Modular Generator	σ_R	σ_I	ϕ	τ	l
I_a	$\mathbf{I}$	1	τ	$-\pi\tau$	τ	$\tilde{l}$	I_c	$\mathbf{P}$	1	τ	π	τ	$\tilde{l}$
I_b	$\mathbf{S}$	$\frac{1}{\tau}$	1	$-\pi$	$-\frac{1}{\tau}$	$\tilde{l}'$	I_d	$\mathbf{SP}$	$\frac{1}{\tau}$	1	$\frac{\pi}{\tau}$	$-\frac{1}{\tau}$	$\tilde{l}'$
III_a	$\mathbf{T}$	1	τ	$-\pi\tau$	$\tau+1$	$\mathrm{i}\frac{\tilde{l}}{\tilde{l}'}$	III_c	$\mathbf{TP}$	1	τ	π	$\tau+1$	$\mathrm{i}\frac{\tilde{l}}{\tilde{l}'}$
II_b	$\mathbf{TS}$	$\frac{1}{\tau}$	1	$-\pi$	$\frac{\tau-1}{\tau}$	$\frac{1}{\tilde{l}'}$	II_d	$\mathbf{TSP}$	$\frac{1}{\tau}$	1	$\frac{\pi}{\tau}$	$\frac{\tau-1}{\tau}$	$\frac{1}{\tilde{l}'}$
III_b	$\mathbf{ST}$	$\frac{1}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{-\pi\tau}{\tau+1}$	$\frac{-1}{\tau+1}$	$\mathrm{i}\frac{\tilde{l}'}{\tilde{l}}$	III_d	$\mathbf{STP}$	$\frac{1}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{\pi}{\tau+1}$	$\frac{-1}{\tau+1}$	$\mathrm{i}\frac{\tilde{l}'}{\tilde{l}}$
II_a	$\mathbf{TST}$	$\frac{1}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{-\pi\tau}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{1}{\tilde{l}}$	II_c	$\mathbf{TSTP}$	$\frac{1}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{\pi}{\tau+1}$	$\frac{\tau}{\tau+1}$	$\frac{1}{\tilde{l}}$
	$\mathbf{STS}$	$\frac{1}{\tau-1}$	$\frac{\tau}{\tau-1}$	$\frac{-\pi\tau}{\tau-1}$	$\frac{\tau}{\tau-1}$	$\frac{1}{\tilde{l}}$		$\mathbf{STSP}$	$\frac{1}{\tau-1}$	$\frac{\tau}{\tau-1}$	$\frac{\pi}{\tau-1}$	$\frac{\tau}{\tau-1}$	$\frac{1}{\tilde{l}}$

Table 1. List of the action of modular transformations, according to (23, 29), in mapping the phase diagram, starting from I_a with the parametrization given by (22)

generate a $\mathbb{Z}_2$-extension that can be identified with $PGL(2,\mathbb{Z})$. These are the same group laws satisfied by the generators of the symmetries of the XYZ chain, as discussed in the introduction.

We collect in table 1 the action of the different transformations generated by $\mathbf{T}$, $\mathbf{S}$ and $\mathbf{P}$ in mapping region I_a in the rest of the phase diagram. It is clear that $\mathfrak{G}$ is isomorphic to the group generated by $\tilde{\mathbf{R}}_{y,z}$, $\tilde{\mathbf{R}}_{x,z}$, and $\tilde{\mathbf{P}}_{y,z}$, as we anticipated, and thus, for instance, $\mathbf{S}\cdot\mathbf{T} = \tilde{\mathbf{R}}_{y,z}\cdot\tilde{\mathbf{R}}_{x,z} = \mathbf{R}_{x,z}\cdot\mathbf{R}_{y,z}$. A few additional comments are in order. In the previous section we gave a prescription for the path of the argument around a rectangle, see (20) and figure 3. This structure is explained by table 1: the $\mathbf{S}$ generator interchanges the role of the axes and thus the path that runs along the imaginary axis in the new basis runs along the real one, consistently with the prescription given for regions of type b and d. The action of $\mathbf{P}$ is to shift the path and thus interchanges regions of type a with c and b with d (and viceversa). The role of $\mathbf{P}$ can be thought of as that of promoting the modular group to its discrete affine.

In conclusions, we see that the whole line $l^2 \in (-\infty,\infty)$ can be used in (20), which divides in three parts, one for each of the regions of type I, II, or III. It is known, that, for each point on this line, only if the argument of the elliptic functions is purely imaginary or purely real (modulo a half periodicity) we are guaranteed that the parameters of the model are real. Hence the two (four) paths, related by $\mathbf{S}$ (and $\mathbf{P}$) duality. The paths of the argument are compact, due to periodicity. Thus, the mapping between (u,l) and (J_y,J_z) is topologically equivalent to $\mathbb{R}^2 \to \mathbb{R}\otimes\mathbb{C}\otimes\mathbb{Z}_2\otimes\mathbb{Z}_2$. Extending the mapping by considering a generic complex argument u, would yield a non-hermitian Hamiltonian, but would preserve the structure that makes it integrable. We do not have a physical interpretation for such a non-unitary extension, but its mathematical

properties indicates that it might be worth exploring this possibility.

6. Conclusions and outlooks

The possibility to write an exact solution for the XYZ spin chain is based on its relation with the eight-vertex model. However, the relation between the parameters (Γ, Δ) of the latter is not one to one with the couplings (J_x, J_y, J_z) of the former (and with the Boltzmann weights of the classical model as well): indeed such mapping changes in the different regions of the phase diagram, see eq.ns (6, 7). In this paper, we have shown that this re-arrangement procedure can be reproduced by means of the *natural* analytical extension of the solution valid in a given initial region. We have also given a prescription that relates the parameter (u, l) of the elliptic functions and the physical parameter of the XYZ model in the whole of the phase diagram and provided an inversion formula valid everywhere.

Clearly symmetries in the space of parameters become manifest as invariance properties of observables and correlations. For example, in [9] we have analytically calculated entanglement entropies for the XYZ model and in particular obtained an expression for the corrections to the leading terms of Rényi entropies that emerge as soon as one moves into the massive region, starting from the critical (conformal) line. Also, by making explicit use of such a kind of parametrization, we have shown that finite size and finite mass effects give rise to different contributions (with different exponents), thus violating simple scaling arguments. This topic deserves further analytical and numerical studies that we plan to present in a future paper.

The main novelty of the approach presented in this paper lies in the connection between analytic continuation in the parameter space and the action of the modular group. This connection allowed us to show that a certain extension of the modular group realizes in parameter space the physical symmetries of the model. This symmetries are in the form of *dualities*, since they connect points with different coupling, related by some spin rotation.

Modular invariance plays a central role in the structure and integrability of Conformal Field Theories in $1 + 1$ dimension. On its critical lines, the XYZ model is described by a $c = 1$ CFT and thus, in the scaling limit, its partition function is modular invariant in real space. Our results show that, even in the gapped phase, it is also a modular invariant in parameter space, due to the symmetries of the model. Elliptic structures are common in the solution of integrable models and it is tempting to speculate that their modular properties do encode in general their symmetries and thus the class of integrability-preserving relevant perturbations that drive the system away from criticality.

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Appendix A. Elliptic Functions

Elliptic functions are the extensions of the trigonometric functions to work with doubly periodic expressions, i.e. such that

$$f\left(z+2n\omega_1+2m\omega_3\right)=f\left(z+2n\omega_1\right)=f(z)\;, \tag{A.1}$$

where ω_1, ω_3 are two different complex numbers and n, m are integers (following [21], we have $\omega_1+\omega_2+\omega_3=0$).

The Jacobi elliptic functions are usually defined through the pseudo-periodic *theta functions*:

$$\theta_1(z;q)=2\sum_{n=0}^{\infty}(-1)^n q^{(n+1/2)^2}\sin[(2n+1)z]\;, \tag{A.2a}$$

$$\theta_2(z;q)=2\sum_{n=0}^{\infty}q^{(n+1/2)^2}\cos[(2n+1)z]\;, \tag{A.2b}$$

$$\theta_3(z;q)=1+2\sum_{n=1}^{\infty}q^{n^2}\cos(2nz)\;, \tag{A.2c}$$

$$\theta_4(z;q)=1+2\sum_{n=1}^{\infty}(-1)^n q^{n^2}\cos(2nz)\;, \tag{A.2d}$$

where the *elliptic nome* q is usually written as $q\equiv \mathrm{e}^{\mathrm{i}\pi\tau}$ in terms of the elliptic parameter τ and accordingly

$$\theta_j(z|\tau)\equiv\theta_j(z;q)\;. \tag{A.3}$$

The periodicity properties of the theta functions are

$$\theta_1(z|\tau)=-\theta_1(z+\pi|\tau)=-\lambda\theta_1(z+\pi\tau|\tau)=\lambda\theta_1(z+\pi+\pi\tau|\tau)\;, \tag{A.4a}$$

$$\theta_2(z|\tau)=-\theta_2(z+\pi|\tau)=\lambda\theta_2(z+\pi\tau|\tau)=-\lambda\theta_2(z+\pi+\pi\tau|\tau)\;, \tag{A.4b}$$

$$\theta_3(z|\tau)=\theta_3(z+\pi|\tau)=\lambda\theta_3(z+\pi\tau|\tau)=\lambda\theta_3(z+\pi+\pi\tau|\tau)\;, \tag{A.4c}$$

$$\theta_4(z|\tau)=\theta_4(z+\pi|\tau)=-\lambda\theta_4(z+\pi\tau|\tau)=-\lambda\theta_4(z+\pi+\pi\tau|\tau)\;, \tag{A.4d}$$

where $\lambda\equiv q\mathrm{e}^{2\mathrm{i}z}$.

Moreover, incrementation of z by the half periods $\frac{1}{2}\pi, \frac{1}{2}\pi\tau$, and $\frac{1}{2}\pi(1+\tau)$ leads to

$$\theta_1(z|\tau)=-\theta_2(z+\tfrac{1}{2}\pi|\tau)=-\mathrm{i}\mu\theta_4(z+\tfrac{1}{2}\pi\tau|\tau)=-\mathrm{i}\mu\theta_3(z+\tfrac{1}{2}\pi+\tfrac{1}{2}\pi\tau|\tau)\;, \tag{A.5a}$$

$$\theta_2(z|\tau)=\theta_1(z+\tfrac{1}{2}\pi|\tau)=\mu\theta_3(z+\tfrac{1}{2}\pi\tau|\tau)=\mu\theta_4(z+\tfrac{1}{2}\pi+\tfrac{1}{2}\pi\tau|\tau)\;, \tag{A.5b}$$

$$\theta_3(z|\tau)=\theta_4(z+\tfrac{1}{2}\pi|\tau)=\mu\theta_2(z+\tfrac{1}{2}\pi\tau|\tau)=\mu\theta_1(z+\tfrac{1}{2}\pi+\tfrac{1}{2}\pi\tau|\tau)\;, \tag{A.5c}$$

$$\theta_4(z|\tau)=\theta_3(z+\tfrac{1}{2}\pi|\tau)=-\mathrm{i}\mu\theta_1(z+\tfrac{1}{2}\pi\tau|\tau)=\mathrm{i}\mu\theta_2(z+\tfrac{1}{2}\pi+\tfrac{1}{2}\pi\tau|\tau)\;, \tag{A.5d}$$

with $\mu \equiv q^{1/4} \mathrm{e}^{\mathrm{i}z}$.

The Jacobi elliptic functions are then defined as

$$\mathrm{sn}(u;k) = \frac{\theta_3(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_1(z|\tau)}{\theta_4(z|\tau)} , \tag{A.6a}$$

$$\mathrm{cn}(u;k) = \frac{\theta_4(0|\tau)}{\theta_2(0|\tau)} \frac{\theta_2(z|\tau)}{\theta_4(z|\tau)} , \tag{A.6b}$$

$$\mathrm{dn}(u;k) = \frac{\theta_4(0|\tau)}{\theta_3(0|\tau)} \frac{\theta_3(z|\tau)}{\theta_4(z|\tau)} , \tag{A.6c}$$

where $u = \theta_3^2(0|\tau)\, z = \frac{2}{\pi} K(k)\, z$, $\tau \equiv \mathrm{i} \frac{K(k')}{K(k)}$, $k' \equiv \sqrt{1-k^2}$, and

$$K(k) \equiv \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-k^2t^2)}} = \int_0^{\frac{\pi}{2}} \frac{\mathrm{d}\theta}{\sqrt{1-k^2\sin^2\theta}} \tag{A.7}$$

is the elliptic integral of the first type. Additional elliptic functions can be generated with the following two rules: denote with p, q the letters s, n, c, d, then

$$\mathrm{pq}(u;k) \equiv \frac{1}{\mathrm{qp}(u;k)} , \qquad \mathrm{pq}(u;k) \equiv \frac{\mathrm{pn}(u;k)}{\mathrm{qn}(u;k)} . \tag{A.8}$$

For $0 \le k \le 1$, $K(k)$ is real, $\mathrm{i}K'(k) \equiv \mathrm{i}K(k')$ is purely imaginary and together they are called *quater-periods*. The Jacobi elliptic functions inherit their periodic properties from the theta functions, thus:

$$\mathrm{sn}(u;k) = -\,\mathrm{sn}(u+2K;k) = \mathrm{sn}(u+2\mathrm{i}K';k) = -\mathrm{sn}(u+2K+2\mathrm{i}K';k) , \tag{A.9a}$$

$$\mathrm{cn}(u;k) = -\,\mathrm{cn}(u+2K;k) = -\mathrm{cn}(u+2\mathrm{i}K';k) = \mathrm{cn}(u+2K+2\mathrm{i}K';k) , \tag{A.9b}$$

$$\mathrm{dn}(u;k) = \mathrm{dn}(u+2K;k) = -\mathrm{dn}(u+2\mathrm{i}K';k) = -\mathrm{dn}(u+2K+2\mathrm{i}K';k) . \tag{A.9c}$$

The inverse of an elliptic function is an elliptic integral. The *incomplete elliptic integral of the first type* is usually written as

$$F(\phi;k) = \int_0^{\phi} \frac{\mathrm{d}\theta}{\sqrt{1-k^2\sin^2\theta}} = \mathrm{sn}^{-1}(\sin\phi;k) , \tag{A.10}$$

and it is the inverse of the elliptic sn. Clearly, $F\left(\frac{\pi}{2};k\right) = K(k)$. Further inversion formulae for the elliptic functions can be found in [21].

Additional important identities include

$$k = k(\tau) = \frac{\theta_2^2(0|\tau)}{\theta_3^2(0|\tau)} , \qquad k' = k'(\tau) = \frac{\theta_4^2(0|\tau)}{\theta_3^2(0|\tau)} , \tag{A.11}$$

and

$$\mathrm{sn}^2(u;k) + \mathrm{cn}^2(u;k) = 1 , \tag{A.12}$$

$$\mathrm{dn}^2(u;k) + k^2\mathrm{sn}^2(u;k) = 1 , \tag{A.13}$$

$$\mathrm{dn}^2(u;k) - k^2\mathrm{cn}^2(u;k) = k'^2 . \tag{A.14}$$

Taken together, the elliptic functions have common periods $2\omega_1 = 4K(k)$ and $2\omega_3 = 4\mathrm{i}K'(k)$. These periods draw a lattice in $\mathbb{C}$, which has the topology of a torus. While the

natural domain is given by the rectangle with corners $(0,0),(4K,0),(4K,4\mathrm{i}K'),(0,4\mathrm{i}K')$, any other choice would be exactly equivalent. Thus, the parallelogram defined by the half-periods

$$\omega_1' = a\,\omega_1 + b\,\omega_3\;, \qquad \omega_3' = c\,\omega_1 + d\,\omega_3\;, \tag{A.15}$$

with a,b,c,d integers such that $ad-bc=1$, can suit as a fundamental domain. This transformation, which also changes the elliptic parameter as

$$\tau' = \frac{\omega_3'}{\omega_1'} = \frac{c+d\,\tau}{a+b\,\tau}\;, \tag{A.16}$$

can be casted in a matrix form as

$$\begin{pmatrix} \omega_1' \\ \omega_3' \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_3 \end{pmatrix} \tag{A.17}$$

and defines a *modular transformation*. The modular transformations generate the *modular group* $\mathrm{PSL}(2,\mathbb{Z})$. Each element of this group can be represented (in a **not** unique way) by a combination of the two transformations

$$\mathbf{S} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \longrightarrow \qquad \tau' = -\frac{1}{\tau}\;, \tag{A.18}$$

$$\mathbf{T} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \qquad \longrightarrow \qquad \tau' = \tau + 1\;, \tag{A.19}$$

which satisfy the defining relations

$$\mathbf{S}^2 = \mathbf{1}\;, \qquad (\mathbf{ST})^3 = \mathbf{1}\;. \tag{A.20}$$

The transformation properties for the $\mathbf{S}$ transformation are

$$\theta_1\left(z|-\frac{1}{\tau}\right) = -\,\mathrm{i}(\mathrm{i}\tau)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}\tau z^2}{\pi}}\theta_1(\tau z|\tau)\;, \tag{A.21a}$$

$$\theta_2\left(z|-\frac{1}{\tau}\right) = (-\mathrm{i}\tau)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}\tau z^2}{\pi}}\theta_4(\tau z|\tau)\;, \tag{A.21b}$$

$$\theta_3\left(z|-\frac{1}{\tau}\right) = (-\mathrm{i}\tau)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}\tau z^2}{\pi}}\theta_3(\tau z|\tau)\;, \tag{A.21c}$$

$$\theta_4\left(z|-\frac{1}{\tau}\right) = (-\mathrm{i}\tau)^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}\tau z^2}{\pi}}\theta_2(\tau z|\tau)\;. \tag{A.21d}$$

From which follows

$$k\left(-\frac{1}{\tau}\right) = k'(\tau)\;, \qquad k'\left(-\frac{1}{\tau}\right) = k(\tau)\;, \tag{A.22}$$

and

$$K\left(-\frac{1}{\tau}\right) = K'(\tau) = K(k')\;, \qquad \mathrm{i}K'\left(-\frac{1}{\tau}\right) = \mathrm{i}K(\tau) = \mathrm{i}K(k)\;. \tag{A.23}$$

Moreover,

$$\mathrm{sn}(u;k') = -\mathrm{i}\frac{\mathrm{sn}(\mathrm{i}u;k)}{\mathrm{cn}(\mathrm{i}u;k)}\,, \qquad \mathrm{cn}(u;k') = \frac{1}{\mathrm{cn}(\mathrm{i}u;k)}\,,$$
$$\mathrm{dn}(u;k') = \frac{\mathrm{dn}(\mathrm{i}u;k)}{\mathrm{cn}(\mathrm{i}u;k)}\,, \qquad \ldots \tag{A.24}$$

For the $\mathbf{T}$ transformation we have

$$\theta_1\left(z|\tau+1\right) = \mathrm{e}^{\mathrm{i}\pi/4}\theta_1(z|\tau)\,, \tag{A.25a}$$
$$\theta_2\left(z|\tau+1\right) = \mathrm{e}^{\mathrm{i}\pi/4}\theta_2(z|\tau)\,, \tag{A.25b}$$
$$\theta_3\left(z|\tau+1\right) = \theta_4(z|\tau)\,, \tag{A.25c}$$
$$\theta_4\left(z|\tau+1\right) = \theta_3(z|\tau)\,, \tag{A.25d}$$

and thus

$$k(\tau+1) = \mathrm{i}\frac{k(\tau)}{k'(\tau)}\,, \qquad k'(\tau+1) = \frac{1}{k'(\tau)}\,, \tag{A.26}$$

and

$$K(\tau+1) = k'(\tau)K(\tau)\,, \qquad \mathrm{i}K'(\tau+1) = k'\left[K(\tau)+\mathrm{i}K'(\tau)\right]\,. \tag{A.27}$$

Finally

$$\mathrm{sn}\left(u;\mathrm{i}\frac{k}{k'}\right) = k - \frac{\mathrm{sn}(u/k';k)}{\mathrm{dn}(u/k';k)}\,, \quad \mathrm{cn}\left(u;\mathrm{i}\frac{k}{k'}\right) = \frac{\mathrm{cn}(u/k';k)}{\mathrm{dn}(u/k';k)}\,,$$
$$\mathrm{dn}\left(u;\mathrm{i}\frac{k}{k'}\right) = \frac{1}{\mathrm{dn}(u/k';k)}\,, \qquad \ldots \tag{A.28}$$

While it is true that by composing these two transformations we can generate the whole group, for convenience we collect here the formulae for another transformation we use in the body of the paper: $\tau \to \frac{\tau}{1-\tau}$, corresponding to **STS**

$$\theta_1\left(z|\frac{\tau}{1-\tau}\right) = \mathrm{i}^{\frac{1}{2}}F\,\theta_1\Big((1-\tau)z|\tau\Big)\,, \tag{A.29a}$$
$$\theta_2\left(z|\frac{\tau}{1-\tau}\right) = F\,\theta_3\Big((1-\tau)z|\tau\Big)\,, \tag{A.29b}$$
$$\theta_3\left(z|\frac{\tau}{1-\tau}\right) = F\,\theta_2\Big((1-\tau)z|\tau\Big)\,, \tag{A.29c}$$
$$\theta_4\left(z|\frac{\tau}{1-\tau}\right) = \mathrm{i}^{\frac{1}{2}}F\,\theta_4\Big((1-\tau)z|\tau\Big)\,, \tag{A.29d}$$

where $F = (1-\tau)^{\frac{1}{2}}\mathrm{e}^{\mathrm{i}\frac{(\tau-1)z^2}{\pi}}$. We have

$$k\left(\frac{\tau}{1-\tau}\right) = \frac{1}{k(\tau)} = \frac{1}{k}\,, \qquad k'\left(\frac{\tau}{1-\tau}\right) = \mathrm{i}\frac{k'(\tau)}{k(\tau)} = \mathrm{i}\frac{k'}{k}\,, \tag{A.30}$$

and

$$K\left(\frac{\tau}{1-\tau}\right) = k\left[K(\tau)-\mathrm{i}K'(\tau)\right]\,, \qquad \mathrm{i}K'\left(\frac{\tau}{1-\tau}\right) = \mathrm{i}kK'(\tau)\,. \tag{A.31}$$

Moreover,

$$
\begin{aligned}
&\mathrm{sn}\left(u;\frac{1}{k}\right) = k\,\mathrm{sn}\left(\frac{u}{k};k\right)\;, \qquad \mathrm{cn}\left(u;\frac{1}{k}\right) = \mathrm{dn}\left(\frac{u}{k};k\right)\;, \\
&\mathrm{dn}\left(u;\frac{1}{k}\right) = \mathrm{cn}\left(\frac{u}{k};k\right)\;, \qquad \ldots
\end{aligned}
\tag{A.32}
$$

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